

# Quantum Simulations of Classical Annealing Processes

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We describe a quantum algorithm that solves combinatorial optimization problems by quantum simulation of a classical simulated annealing process. Our algorithm exploits quantum walks and the quantum Zeno effect induced by evolution randomization. It requires order  $1/\sqrt{\delta}$  steps to find an optimal solution with bounded error probability, where  $\delta$  is the minimum spectral gap of the stochastic matrices used in the classical annealing process. This is a quadratic improvement over the order  $1/\delta$  steps required by the latter.

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Combinatorial optimization problems (COPs) are important in almost every branch of science, from computer science to statistical physics and computational biology [1]. Each instance of a COP requires that we minimize some objective function over a search space consisting of  $d$  configurations. The search space may have additional structure, such as that provided by a graph, to give a notion of locality. Because  $d$  is typically exponential in the size of the problem instance, finding a solution by exhaustive search is hard in general. One can exploit the notion of locality to find solutions more quickly, but the presence of many nonoptimal local minima often prevents efficient convergence to a solution. Therefore, more efficient optimization strategies are desirable.

A well known and often used general strategy for solving COPs is simulated annealing (SA) [2]. SA imitates the process undergone by a metal that is heated to a high temperature and then cooled slowly enough for thermal excitations to prevent it from getting stuck in local minima, so that it ends up in one of its lowest-energy configurations. In SA, the objective function  $E$  of the COP plays the role of the energy, so the lowest energy configuration is the optimum. The annealing process can be simulated with a variety of techniques. Here, we focus on discrete Markov chain Monte-Carlo (MCMC) as used, for example, in statistical physics [3]. MCMC generates a stochastic sequence of configurations via a Markov process that, in the case of SA, converges to the Gibbs distribution at a low final temperature. More specifically, the annealing process is determined by a choice of an *annealing schedule* consisting of a finite increasing sequence of *inverse temperatures*  $\beta_1 < \beta_2 < \dots < \beta_P$ , and by an associated sequence of *transition rules*  $\{M_1, \dots, M_P\}$  consisting of stochastic matrices acting on configurations. When the structure of the problem can be exploited by a good choice of transition rules, the MCMC algorithm can outperform exhaustive search.

One way to characterize the implementation complexity of SA based on MCMC is to count the number of times that the transition rules must be applied before converging to the desired final distribution within an acceptable error. For simplicity, we consider regular annealing schedules with  $\beta_k = (k-1)\Delta\beta$  and choose  $\Delta\beta = \mathcal{O}(\delta/E_M)$ , where  $\delta$  is the minimum spectral gap of the matrices  $M_k$  and  $E_M = \max_{\sigma} |E[\sigma]|$ . We assume that  $E$  has been shifted so that  $E \geq 0$ . Let  $\gamma$  be the spectral gap of  $E$ , defined as the difference between the two smallest values in the range of  $E$ . By adapting arguments from Ref. [4] to the discrete-time setting it can be shown that if  $\beta_P = P\Delta\beta = \mathcal{O}(\gamma^{-1} \log(d/\epsilon^2))$ , then the probability that SA does not return an optimal configuration is no greater than  $\epsilon$ . Thus, for a success probability greater than  $1 - \epsilon$ , the implementation complexity of SA is given by  $\mathcal{N}_{SA} = P = \mathcal{O}\left(\frac{E_M}{\gamma} \log(d/\epsilon^2)/\delta\right)$ .

Ideally,  $\mathcal{N}_{SA}$  is small compared to the size  $d$  of the configuration space. Since problem instance sizes are typically polylogarithmic in  $d$ ,  $\mathcal{N}_{SA} = \mathcal{O}(\text{polylog}(d))$  is considered efficient. Efficient  $\mathcal{N}_{SA}$  is obtained, for example, when computing physical properties of the  $N$ -spin ferromagnetic Ising model in an homogeneous external field [5]. However, inefficient  $\mathcal{N}_{SA}$  is obtained if the external field is random [6], making the problem intractable due to gaps  $\delta$  that are exponentially small in  $N$ . The dependence of the complexity of MCMC on  $\delta^{-1}$  is characteristic of Markov processes and may be unavoidable [7]. Thus, finding new methods with better scaling in  $\delta$  is very desirable.

Quantum mechanics provides new resources with which to attack optimization problems [8, 9]. Quantum computers (QCs) can theoretically solve some problems, including integer number factorization and unstructured search, more efficiently than classical computers [10]. Still, whether a QC could solve all COPs more efficiently than is possible with classical computers is an open question. In this Letter we show that QCs can speed up the simulation of classical annealing processes. We present a method for transforming instances of MCMC-based SA

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into a quantum simulated annealing (QSA) algorithm for which the number of times,  $\mathcal{N}_{QSA}$ , that the transition rules are used is  $\mathcal{O}((E_M/\gamma)^2 \log^2(d/\epsilon) \log d/(\epsilon\sqrt{\delta}))$ , a quadratic improvement as a function of  $\delta^{-1}$ . This improvement is most significant for hard instances where  $\delta \ll 1$ . The dependence on  $1/\epsilon$  can be improved to  $\text{polylog}(1/\epsilon)$ . QSA is based on ideas and techniques from quantum walks [11] and the quantum Zeno effect, where the latter can be implemented by phase estimation or by randomization of an evolution period.

This paper is organized as follows. First we describe a “quantization” of a reversible, ergodic Markov chain in terms of a bipartite quantum walk. This is a similarity-transformed version of the quantum walk used in Refs. [11] to obtain quantum speedups in search problems. The quantum walk is a unitary operator acting on the state space obtained by superposition from the configurations of the COP. We then explain how to transform an instance of SA by adapting the annealing schedule and applying the Markov chain quantization. Finally, we analyze the complexity of QSA to determine the speedup over SA.

**Quantum Walks and Markov Chains.** Discrete-time quantum walks were introduced as the quantum analogues of classical random walks [12]. We focus on the bipartite quantum walks defined in Refs. [11].

Consider a  $d$ -configuration classical system  $\mathcal{S}$  with energies  $E[\sigma]$  for configurations  $\sigma$ . Denote the space of ground configurations (minimizers of  $E$ ) by  $\mathbb{S}_0$ . Consider an ergodic, reversible Markov process on  $\mathcal{S}$  with transition probabilities  $p(\sigma'|\sigma) = m_{\sigma\sigma'}$  and stationary distribution  $\pi^\sigma$ . Reversibility is equivalent to the detailed balance condition  $\pi^\sigma m_{\sigma\sigma'} = \pi^{\sigma'} m_{\sigma'\sigma}$ . Let  $\mathcal{H}$  be the quantum state space spanned by orthonormal states  $|\sigma\rangle$  for configurations  $\sigma$  of  $\mathcal{S}$ . In SA,  $\pi^\sigma = e^{-\beta E[\sigma]}/\mathcal{Z}$  with  $\mathcal{Z} = \sum_\sigma e^{-\beta E[\sigma]}$  is the Gibbs distribution at some inverse temperature  $\beta$ . We assume not only that we have a classical algorithm to efficiently sample from the distribution  $m_{\sigma\sigma'}$  given  $\sigma$ , but also that we have an efficient quantum algorithm that computes the transformation defined by  $|\sigma\rangle|\mathbf{o}\rangle \mapsto |\sigma\rangle \sum_{\sigma'} \sqrt{m_{\sigma\sigma'}} |\sigma'\rangle$ , with  $|\mathbf{o}\rangle$  an efficiently preparable state of  $\mathcal{H}$  (e.g. a computational basis state). Note that this stronger condition is usually satisfied, because for given  $\sigma$ ,  $m_{\sigma\sigma'}$  is non-zero for only polynomially many  $\sigma'$ , and the non-zero  $m_{\sigma\sigma'}$  can be computed efficiently by a classical algorithm.

The bipartite quantum walk is defined on the tensor product  $\mathcal{H}_A \otimes \mathcal{H}_B$  of two copies of  $\mathcal{H}$ . Following [11], we define isometries  $X$  and  $Y$  that map states of  $\mathcal{H}$  to states of  $\mathcal{H}_A \otimes \mathcal{H}_B$  by

$$X|\sigma\rangle = |\sigma\rangle \sum_{\sigma'} \sqrt{m_{\sigma\sigma'}} |\sigma'\rangle, \quad (1)$$

$$Y|\sigma'\rangle = \sum_{\sigma} \sqrt{m_{\sigma'\sigma}} |\sigma\rangle |\sigma'\rangle. \quad (2)$$

Let  $D_\pi$  be the diagonal matrix with entries  $\pi^\sigma$  on the diagonal. Let  $M$  be the matrix with entries  $M_{\sigma'\sigma} =$

$m_{\sigma\sigma'}$ . From the detailed balance condition,  $X^\dagger Y = D_\pi^{1/2} M D_\pi^{-1/2}$  is symmetric. It follows that  $X^\dagger Y$  and  $M$  have the same eigenvalues  $\lambda_0 = 1 > \lambda_1 \geq \dots \geq \lambda_{d-1} \geq 0$ . Let  $|\phi_j\rangle$  be the  $\lambda_j$  eigenstate of  $X^\dagger Y$ . Then  $|\phi_0\rangle = \sum_\sigma \sqrt{\pi^\sigma} |\sigma\rangle$ , which upon measurement in the basis  $|\sigma\rangle$  has the same probability distribution as the stationary distribution of the Markov process.

Define unitary operators  $U_X$  and  $U_Y$  by

$$U_X|\sigma\rangle|\mathbf{o}\rangle \equiv X|\sigma\rangle, \quad U_Y|\mathbf{o}\rangle|\sigma\rangle \equiv Y|\sigma\rangle, \quad (3)$$

with arbitrary action on other states. Let  $P_1$  and  $P_2$  be the projectors onto the subspaces spanned by  $\{|\sigma\rangle|\mathbf{o}\rangle\}_\sigma$  and  $\{U_X^\dagger U_Y|\mathbf{o}\rangle|\sigma\rangle\}_\sigma$ , respectively. The reflection operators through  $P_i$  are defined by  $R_i = 2P_i - \mathbb{1}$ . A step of the bipartite quantum walk  $W$  based on  $M$  is given by  $W = R_2 R_1$ . This walk is related to the one used in Ref. [11] by a unitary, but  $\pi^\sigma$ -dependent, similarity transformation, which helps avoid amplitude leakage when  $W$  changes in QSA.

The spectrum of  $W$  is directly related to the spectrum of  $M$  [11]. Define phases  $\varphi_j = \arccos \lambda_j$ , so that  $X^\dagger Y|\phi_j\rangle = \cos \varphi_j |\phi_j\rangle$ . The spectral gap of  $M$  is  $\delta = 1 - \lambda_1 \leq (\varphi_1)^2/2$ . From Eq. (3),

$$P_1 U_X^\dagger U_Y|\mathbf{o}\rangle|\phi_j\rangle = \cos \varphi_j |\phi_j\rangle|\mathbf{o}\rangle \quad (4)$$

$$P_2 |\phi_j\rangle|\mathbf{o}\rangle = \cos \varphi_j U_X^\dagger U_Y|\mathbf{o}\rangle|\phi_j\rangle, \quad (5)$$

so  $W$  preserves the (at most) two-dimensional subspace spanned by  $\{|\phi_j\rangle|\mathbf{o}\rangle, U_X^\dagger U_Y|\mathbf{o}\rangle|\phi_j\rangle\}$ . In terms of the Bloch sphere defined by states in this subspace, for  $j \geq 1$ ,  $W$  acts as a  $4\varphi_j$  rotation along an axis perpendicular to the Bloch-sphere directions spanned by the defining states [13]. Thus, the eigenphases of  $W$  in this subspace are  $\pm 2\varphi_j$ . The eigenphase-0 states are either the *quantum stationary state*  $|\psi_0\rangle = |\phi_0\rangle|\mathbf{o}\rangle$  or orthogonal to both  $P_i$ . The goal is to prepare  $|\psi_0\rangle$  so that we can sample from the stationary distribution of  $M$  by measuring the first system. (The preparation of  $|\phi_0\rangle$  and its relation to statistical zero knowledge was studied in [14].)

To compare a quantum algorithm based on uses of  $W$  to the classical Markov chain algorithm, note that  $W$  is readily implemented in terms of four quantum steps, each of whose complexity is closely related to the steps of the classical Markov chain, given our assumptions. For the purpose of asymptotic comparison, it therefore suffices to consider the number of quantum steps  $W$  versus the number of classical steps based on  $M$ .

**Quantum Simulated Annealing.** We assume that for any  $\beta \geq 0$ , there is a transition matrix  $M_\beta$  satisfying the assumptions of the previous section and with stationary distribution  $\pi_\beta^\sigma = e^{-\beta E[\sigma]}/\mathcal{Z}$ . Like SA, QSA is based on an annealing schedule that we choose to consist of equally spaced inverse temperatures  $\beta_k = (k-1)\Delta\beta$  for  $k = 1, \dots, Q$ . Let  $W_k$  be the quantum walk step operator for  $M_{\beta_k}$ ,  $|\psi_0^k\rangle$  its quantum stationary state (*quantum Gibbs state* for  $\beta_k$ ) and  $\varphi_{1,k}$  its phase gap. The goal of QSA is to sequentially prepare  $|\psi_0^{k+1}\rangle$  from  $|\psi_0^k\rangle$  by

means of an approximate projective measurement onto  $|\psi_0^{k+1}\rangle$  [15] realized by a simulated measurement onto the eigenbasis of  $W_{k+1}$ . We assume that the uniform superposition  $|\psi_0^1\rangle$  can be prepared efficiently. If the states  $|\psi_0^k\rangle$  change slowly enough, the state  $|\psi_0^Q\rangle$  can be obtained with high probability of success, due to a version of the quantum Zeno effect. If  $\beta_Q$  is sufficiently large,  $|\psi_0^Q\rangle$  is a good approximation of a uniform superposition of the ground configurations of  $\mathcal{S}$ , so that we can obtain such a ground configuration with high probability by measurement. The complexity of QSA is dominated by the complexity of the simulated measurements, for which we give two strategies, one based on the phase estimation algorithm (PEA) and the other on randomized applications of  $W_k$ . Both strategies' complexities are dominated by  $1/\varphi_{1,k}$ . The quadratic quantum speedup is due to the quadratic increase of  $\varphi_{1,k}$  over the eigenvalue gap of  $M_k$ .

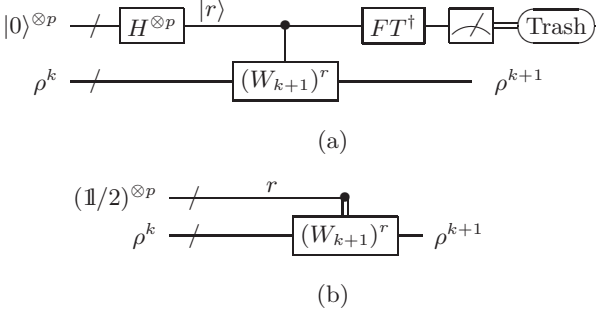


FIG. 1: (a) Phase estimation algorithm. The top  $p$ -qubit register encodes a  $p$ -bit approximation to an eigenphase of  $W_{k+1}$  on readout. The second register's states are in  $\mathcal{H}_A \otimes \mathcal{H}_B$ . The first register is initialized with Hadamard gates to an equal superposition state in the computational basis. A sequence of  $2^p - 1$  controlled  $W_{k+1}$  operations is applied, and the first register is measured after an inverse quantum Fourier transform. If the measurement outcome is  $|0\rangle^{\otimes p}$ , the second register is approximately projected onto a 0-phase eigenstate of  $W_{k+1}$ . (b) Randomization procedure. If the PEA's outcome is ignored, the overall effect on  $\mathcal{H}_A \otimes \mathcal{H}_B$  is equivalent to the one induced by initializing a set of  $p$  bits (first register) in a random state  $r$ , with  $r \in \{0, \dots, 2^p - 1\}$ , and by acting on  $\mathcal{H}_A \otimes \mathcal{H}_B$  with  $(W_{k+1})^r$ . Here, double vertical lines indicate classical control.

The use of PEA in QSA is depicted in Fig. 1(a). QSA does not need to use the result of the phase estimation, though the result could be used to terminate and restart the procedure if the measurement outcome is not  $|0\rangle^{\otimes p}$ . The decoherence it induces in the eigenbasis of  $W_{k+1}$  suffices to achieve the required Zeno effect. Thus, the effect of the PEA on  $\mathcal{H}_A \otimes \mathcal{H}_B$  is equivalent to the one obtained by the action of  $r$   $W_{k+1}$ 's, with  $r$  chosen uniformly at random from 0 to  $2^p - 1$  (Fig. 1(b)). To exponentially reduce the error due to remaining coherences between  $|\psi_0^{k+1}\rangle$  and orthogonal states, we repeat the random process  $s$  times, resulting in a total action of  $W_{k+1}^{\sum_{q=1}^s r_q}$  with  $0 \leq r_q \leq 2^p - 1$  independently random. To prevent ex-

cessive amplitude leakage into undesirable 0-eigenphase eigenstates of  $W_k$ , we decohere the second register after each randomization step. That is, we measure  $\mathcal{H}_B$  in the computational basis and discard the result. The total complexity of QSA is given by  $\mathcal{O}(Q2^p s)$  walk steps, where  $Q$ ,  $p$  and  $s$  are chosen to ensure sufficiently high probability of success.

Let  $\rho^k$  denote the state after the  $k$ 'th randomization and decoherence step. We have  $\rho^1 = |\psi_0^1\rangle\langle\psi_0^1|$ . Assume that  $|\langle\psi_0^{k+1}|\rho^k|\psi_0^{k+1}\rangle| \geq 1 - \mu^2$  for all  $k$ . By expanding to lowest order in  $\Delta\beta$ , one can verify that  $\mu = \mathcal{O}(\Delta\beta E_M)$ . We show by induction that for  $2^p > 2^3\pi/\sqrt{2\delta}$  and  $s \geq 1 + \log_2(2k)/2 = \mathcal{O}(\log(k))$ ,  $\langle\psi_0^k|\rho^k|\psi_0^k\rangle \geq 1 - 2k\mu^2$ . Thus, if  $\mu^2 < \epsilon/(4Q)$ ,  $\rho^Q$  is the quantum Gibbs state for  $\beta = Q\Delta\beta$  with error probability at most  $\epsilon/2$ . We can write  $\rho^k = (1 - \chi)|\psi_0^k\rangle\langle\psi_0^k| + \nu_k(|\psi_0^k\rangle\langle\psi_\perp^k| + \text{H.c.}) + \chi\rho_\perp$ , where  $|\psi_\perp^k\rangle$  is a unit state orthogonal to  $|\psi_0^k\rangle$ ,  $\rho_\perp$  is a density matrix with support orthogonal to  $|\psi_0^k\rangle$ , and  $\chi \leq 2k\mu^2$ . To make the induction argument possible, we add the induction hypothesis  $\nu_k < \mu/2$ . The induction hypotheses apply to  $\rho^1$  by definition. Note that  $\langle\psi_0^{k+1}|\rho^{k+1}|\psi_0^{k+1}\rangle = \langle\psi_0^{k+1}|\rho^k|\psi_0^{k+1}\rangle$ . We can estimate  $\langle\psi_0^{k+1}|\rho^k|\psi_0^{k+1}\rangle \geq (1 - \chi)|\langle\psi_0^{k+1}|\psi_0^k\rangle|^2 - 2\nu_k|\langle\psi_0^{k+1}|\psi_0^k\rangle||\langle\psi_0^{k+1}|\psi_\perp^k\rangle| + \langle\psi_0^{k+1}|\rho_\perp|\psi_0^{k+1}\rangle \geq (1 - 2k\mu^2)(1 - \mu^2) - 2\nu_k\mu \geq 1 - 2(k+1)\mu^2$ . This establishes the main induction hypothesis for  $k+1$ . Before the randomization step, the density matrix's transition between  $|\psi_0^{k+1}\rangle$  and the orthogonal subspace can be written in the form  $\nu'(|\psi_0^{k+1}\rangle\langle\phi_\perp| + \text{H.c.})$  with unit state  $|\phi_\perp\rangle$  orthogonal to  $|\psi_0^{k+1}\rangle$  and the other 0-eigenphase eigenstates of  $W^{k+1}$ , because the decoherence step ensures that the support of  $P_1$  is preserved by the operator  $\rho^k$ . The estimate on  $\langle\psi_0^{k+1}|\rho^k|\psi_0^{k+1}\rangle$  implies that  $\nu' \leq \sqrt{2(k+1)}\mu$  by positivity of  $\rho^k$  [16]. Because  $|\psi_0^{k+1}\rangle$  is stabilized by  $W_{k+1}$ , the transition is transformed by randomization to  $\nu''(|\psi_0^{k+1}\rangle\langle\phi'_\perp| + \text{H.c.})$  with  $\nu''|\phi'_\perp\rangle = \nu' \left( \frac{1}{2^p} \sum_{r=0}^{2^p-1} W_{k+1}^r \right)^s |\phi_\perp\rangle$ . In the eigenbasis of  $W_{k+1}$ , the entries of  $|\phi'_\perp\rangle$  are multiplied by terms with absolute values  $\left( \frac{1}{2^p} \left| \sum_{r=0}^{2^p-1} e^{ir2\varphi} \right| \right)^s \leq \left( \frac{1}{2^{p-1}|1-e^{i2\varphi}|} \right)^s < \left( \frac{\pi}{2^{p-3}|\varphi|} \right)^s < 2^{-s}$ , since the relevant eigenphases  $2\varphi$  satisfy  $\pi/2 \geq |\varphi| \geq \sqrt{2\delta}$ . Thus, the choice  $s = 1 + \log_2(2(k+1))/2$  ensures that  $\nu'' < \mu/2$ . Because the decoherence step preserves  $|\psi_0^{k+1}\rangle$ , we have  $\nu_{k+1} \leq \nu'' < \mu/2$ . This completes the induction step of the proof.

To determine the order of the number of quantum steps  $\mathcal{N}_{QSA}$  required by QSA, let  $\beta_f$  be the desired final inverse temperature, so that  $\Delta\beta = \beta_f/Q$ . Choose  $Q$  to be a sufficiently large multiple of  $\beta_f^2 E_m^2/\epsilon$ . For optimization, we let  $\beta_f = \ln(d/(2\epsilon))/\gamma = \mathcal{O}(\log(d/\epsilon)/\gamma)$ . According to the bounds at the beginning of the previous paragraph, this ensures that after measuring the final state, the probability of finding a non-optimal configuration is at most  $\epsilon$ , with a contribution of  $\epsilon/2$  from the probability of being orthogonal to  $|\psi_0^Q\rangle$  and  $\epsilon/2$  from

the Gibbs distribution's probability of not being optimal. Because  $2^p = \mathcal{O}(1/\sqrt{\delta})$  and  $s = \mathcal{O}(\log(Q))$ , we find that  $\mathcal{N}_{QSA} = \mathcal{O}(Q \log(Q)/\sqrt{\delta})$  with  $Q = \mathcal{O}(\beta_f^2 E_m^2/\epsilon)$  and  $\beta_f = \mathcal{O}(\log(d/\epsilon)/\gamma)$ . If we anticipate that  $Q > d$ , we can just search every configuration classically to find the optima, so we can bound  $\log(Q) \leq \log(d)$  to simplify

$$\mathcal{N}_{QSA} = \mathcal{O} \left( \left( \frac{E_M}{\gamma} \right)^2 \frac{\log^2(d/\epsilon) \log d}{\epsilon \sqrt{\delta}} \right). \quad (6)$$

The dependence of  $\mathcal{N}_{QSA}$  on  $1/\epsilon$  can be improved to  $\text{polylog}(1/\epsilon)$  by repetition of QSA with an initial target error  $\epsilon = 1/2$  in Eq. (6). For optimization, it suffices to repeat QSA  $\mathcal{O}(\log(\epsilon))$  many times. Another approach that may be used to prepare the desired stationary state with high probability of success is to apply a high-confidence version of the PEA [13] at the end of QSA to project onto  $|\psi_0^Q\rangle$ , the stationary state for inverse temperature  $\beta_f$ . If the projection fails, the algorithm is repeated.

Although the dependence of  $\mathcal{N}_{QSA}$  on  $E_M/\gamma$  is worse than the one appearing in classical SA, it is worth noting that unlike the inverse spectral gap  $1/\delta$ , in many important applications this parameter is bounded by a constant or a polynomial in instance size.

**Conclusions.** We presented a quantum algorithm based on a “quantization” of simulated annealing algorithms implemented with MCMC methods. This quantum simulated annealing (QSA) algorithm forces the state to closely follow a superposition with amplitudes derived

from finite-temperature Gibbs distributions. This is accomplished by either an explicit measurement using phase estimation with quantum walk operators, or by decoherence using random applications of these operators. QSA can be used both for combinatorial optimization and for sampling from a Gibbs distribution for statistical physics applications. In contrast to SA, which scales with  $\mathcal{O}(1/\delta)$ , where  $\delta$  is the minimal spectral gap of the transition matrices, QSA scales with  $\mathcal{O}(1/\sqrt{\delta})$ . Although in general the QSA does not yield a polynomial-resource algorithm, it reduces required resources by an asymptotic exponential factor for the ubiquitous hard cases, where the gap becomes exponentially small in the problem size.

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